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Design of very thin CdTe Solar Cells with high efficiency

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Abstract

After several years without change, First Solar announced in 2011 an efficiency record for CdS/CdTe solar cells set at 17.3%, as confirmed by NREL [1]. This is a significant milestone that demonstrates the ongoing potential of CdTe thin-film solar cells. Then, a question arises on the new limits likely to be achieved for the efficiency of this kind of solar cells. The author [2] had previously predicted that with current technology, the practical limit was around 17.5%, but below 18%. In this work, a systematic study of the expected efficiency evolution as a function of fabrication parameters is made with the help of a new solar cell simulator (wxAMPS) [3]. We start from known parameters, so that the simulated results coincide with a previous reported record efficiency (16.5% under AM1.5 G radiation). Then, we show that as the thickness of the CdTe layer is reduced the efficiency will be increased mostly due to a reduced series resistance. It will be shown that there is an optimum thickness for which the highest efficiency becomes 17.7%, confirming the preceding author's prediction. In addition, it will be shown that the introduction of a ZnTe layer at the back of the solar cell (i. e. with a new device structure: CdS/CdTe/ZnTe) will help reaching even higher efficiencies, for very thin solar cells, above 19.5%. These results should be useful for guiding experimentalists to make more efficient CdTe solar cells.

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CdTe,Thin film, Solar cells, High efficiency

1. INTRODUCTION

Heterojunction II–VI compound solar cells (CdS/CdTe) are currently entering mass production, but still there are ways for improving their performance. The highest CdS/CdTe cell efficiency reported [1] is still not near the theoretical (30%) or the practical limit (above 20%), and various strategies for improvement are currently being considered with low-cost fabrication technologies. The current main

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technical issues of CdTe cells are related to less material usage, more stable back ohmic contact and appropriate window layers.

Polycrystalline CdTe has a high absorption coefficient, above 5×10^5 cm^{-1}, which means that all photons with energy greater than the band-gap (Eg) can be absorbed by a thin layer. Moreover, the thinner the absorber layer, the reduced material usage and the lower the cost of fabrication. However, to inhibit the possible recombination loss at the back contact of ultra-thin CdTe solar cells, a wide band-gap material ZnTe (Eg = 2.26 eV) is needed at the back contact [4, 5], making a CdTe/ZnTe hetero-junction. This wide band-gap material would act as a BSF to reflect the carriers at the CdTe/ZnTe heterojunction and thus would decrease the loss of carriers at the back contact.

On the other hand, numerical models have become important tools for the design of any kind of efficient solar cells. Analytic models of solar cells have been used since the earliest days to improve understanding of the operation and to provide guidance for their design [6, 7]. But, as our understanding has increased, our need for more complex models to provide adequate descriptions of their operation has also increased and, as a consequence, we have to do numerical solutions. To a large extent, numerical solution techniques have removed the need to make simplifying assumptions in order to obtain a solution. The need to push cell efficiency towards the limit requires that we have sophisticated tools for the optimization of existing designs and for the comparison of competing design proposals.

In this work, in order to simulate the above mentioned CdTe solar cell structures we have used wxAMPS. This is a substantially new solar cell simulator for modeling one-dimensional devices composed of various materials [3]. It accepts the same input parameters as AMPS, which is a well-known solar cell simulation tool developed by Fonash et al. at Pennsylvania State University [8], conforms to similar physical principles and numerical descriptions of defects and recombination, and adds the effects of tunneling currents based on two different tunneling models [9, 10]. wxAMPS is written in C++ and includes a number of revisions to the basic algorithm. All the details about this new code can be seen in the paper by Liu, Sun and Rockett [3].

2. SIMULATION OF CdS/CdTe/ZnTe SOLAR CELLS WITH wxAMPS

In fig. 1, the basic cell structure under study is depicted. A very thin (0.1 µm) ZnTe layer is added to a conventional CdS/CdTe solar cell at the back in order to reduce the high back surface recombination velocity (S = 1 x 10^7 cm s^{-1}). The set of the parameters required by wxAMPS for all the materials to be used in the simulated solar cells is given in table I. The standard AM1.5G global solar spectrum was used in all cases. For simplicity, reflectance at the back contact is assumed to be 100% while the front reflectance is assumed to be negligible.

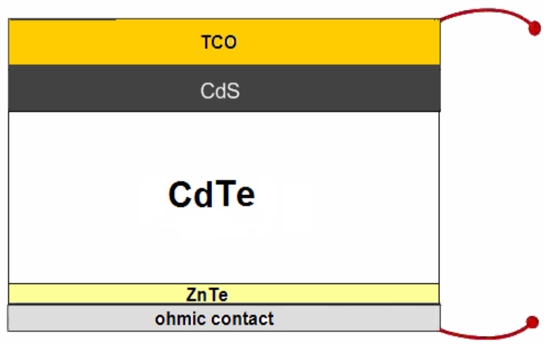

Fig. 1. Proposed CdS/CdTe/ZnTe solar cell structure. The back surface recombination velocity was assumed to be high at the back ohmic contact (S = 1 x 10^6 cm/s). In conventional cells the high back surface recombination limits the efficiency.

Table I. Material parameters used for the simulation with wx-AMPS.

Physical parameters	SnO_2	CdS	CdTe	ZnTe
$\varepsilon/\varepsilon_0$	9	10	9.4	9.4
Eg (eV)	3.6	2.4	1.5	2.15
χ (eV)	4	4	3.9	3.25
μ_n (cm^2 V s^{-1})	100	100	320	820
μ_p (cm^2 V s^{-1})	25	25	40	40
Thickness (nm)	500	50	Variable	100
N_d (cm^{-3})	1×10^{18}	1×10^{18}	----	----
N_a (cm^{-3})	----	----	2.3×10^{14}	1×10^{18}

In the CdTe layer, carrier recombination traps with a (single) Gaussian distribution centered at mid-gap are assumed. The trapping parameters are such that lifetimes are of the order of 5×10^{-10} s, and then the diffusion lengths for minority carriers (electrons) are of the order of 4 μm. This is a value which experimentally will depend on the deposition method and conditions. Unfortunately, researchers reporting high efficiency solar cells usually do not show experimental results for this and other important parameters such as the majority carrier concentration. The majority carrier concentration will be related to the hetero-junction built-in voltage, but it also will determine the electric field distribution in this region.

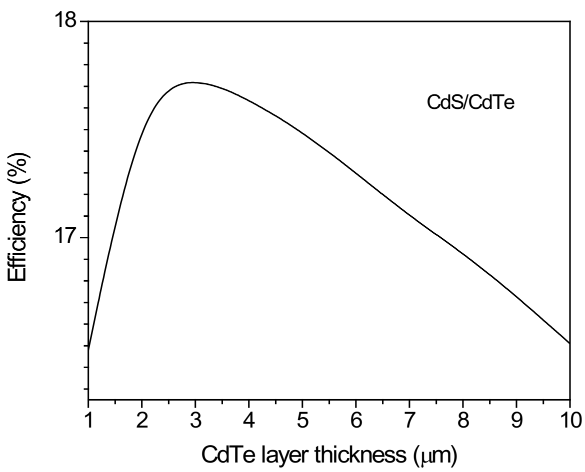

Fig. 2. Solar cell efficiency as a function of CdTe film thickness for the conventional SnO_2/CdS/CdTe structure. This technology would not allow efficiencies higher than 18%. In fact, the maximum would be around 17.7% for optimum CdTe thickness of 3 μm.

Therefore, taking into account this uncertainty, we defined the materials parameters which gave for the conventional structure an efficiency similar to the one obtained by NREL in 2001 [11]. The effect of reducing the CdTe layer thickness upon the efficiency is shown in figure 2. Notice that the efficiency would increase as we decrease the thickness down to 3 μm. This effect is mainly due to the reduction of the associated series resistance which is dominated by the resistivity of the CdTe layer. However, below 3 μm the efficiency falls as a consequence of the reduced photocurrent since the absorption volume is reduced and this effect is higher than the one due to the reduced series resistance. In other words, we expect to have an optimum thickness around 3 μm.

As explained before, the introduction of a ZnTe layer at the back, between the CdTe layer and the back contact will have several effects. The first one is the reduced carrier recombination at the back contact due to the barrier (conduction band discontinuity) for electrons at the interface between the CdTe and the ZnTe layers. This effect can be seen as a **very high back surface electric field** (of the order of 10^5 V/cm) since the potential discontinuity at the CdTe/ZnTe interface is 0.65 V in a very thin interface (transition) region. Then, the electrons will be "reflected" at this interface and they will be collected with a high probability at the CdS/CdTe hetero-junction, so that a high illumination current density will be attained. In addition, the reduced carrier recombination at the back surface will cause a reduced dark saturation current density, so that a high open circuit voltage is also expected.

The second beneficial effect, which will be more of practical importance than a simulation result, is the fact that due to a higher majority carrier concentration in this layer, the ohmic contact at the back will be easier to make and the specific contact resistivity will be reduced as compared to a similar ohmic contact directly on the CdTe layer.

Finally, a third very important effect produced by the back ZnTe layer will be the fact that due to its p+ character, the solar cell will behave as a n-i-p device with a high open circuit voltage since -in this case- Voc will be determined by the total built-in voltage between the CdS and the ZnTe layers. This effect will also be related to the presence of a high electric field in the whole CdTe region (of the order of 10^3 V/cm), and this field will be higher as this layer thickness is reduced. Then, electrons will be drifted by this high electric field towards the CdS/CdTe junction increasing their collection probability. All these effects can be seen in fig. 3 where the band diagram is shown for the case of a solar cell with a 2 μm CdTe layer. The n+ i p+ behavior is apparent in this figure with all the implications mentioned above.

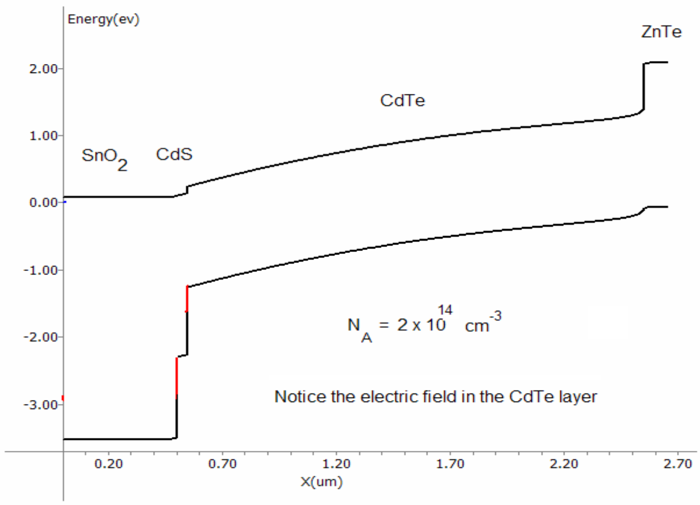

Fig. 3. Band-diagram for the SnO_2/CdS/CdTe/ZnTe solar cell structure with a high resistivity CdTe layer (2 μm). Notice the high electric field in the CdTe layer. Therefore, this structure behaves as an n+ - i – p+ solar cell having a high carrier collection probability and reduced volumetric recombination.

In order to compare with the preceding results for a conventional CdS/CdTe solar cell we calculated the efficiency of the CdS/CdTe/ZnTe solar cell as a function of the CdTe layer thickness. The behavior is similar to the conventional solar cell, except for a small increase of the efficiency as compared to the conventional solar cell down to 3 μm, but below 3 μm the efficiency continues increasing due to the higher carrier collection probability, the reduced dark saturation current density and the reduced series resistance, as shown in fig. 4. The optimum CdTe thickness, in this case, will be smaller than 1 μm, and below this value the reduced absorption will again cause a reduced photo-current and a reduced efficiency. We only show results down to 1 μm because we consider this to be a practical limit, taking into account the fabrication processes which may degrade the performance when the CdTe layer thickness is very thin. For example, if Cu is used as part of the back contact, the thinner the CdTe layer the more likely the shunting of the solar cell is due to Cu diffusion in the CdTe layer. For a 1 μm solar cell the expected efficiency is 19.5% which is higher than the conventional cell with a 10 μm thick CdTe.

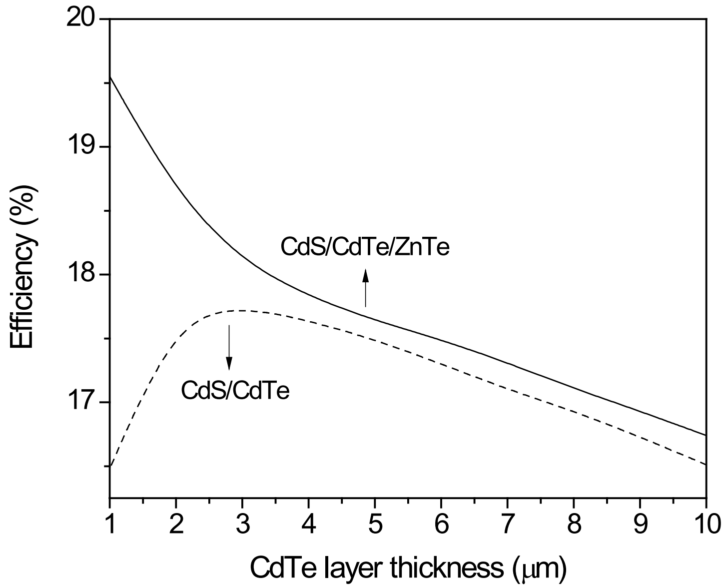

Fig. 4. Solar cell efficiency as a function of CdTe film thickness for $SnO_2/CdS/CdTe/ZnTe$ as compared to the conventional $SnO_2/CdS/CdTe$ structure. The latter technology would not allow efficiencies higher than 18%, but the proposed structure should achieve efficiencies above 19.5%, even for very thin CdTe thickness.

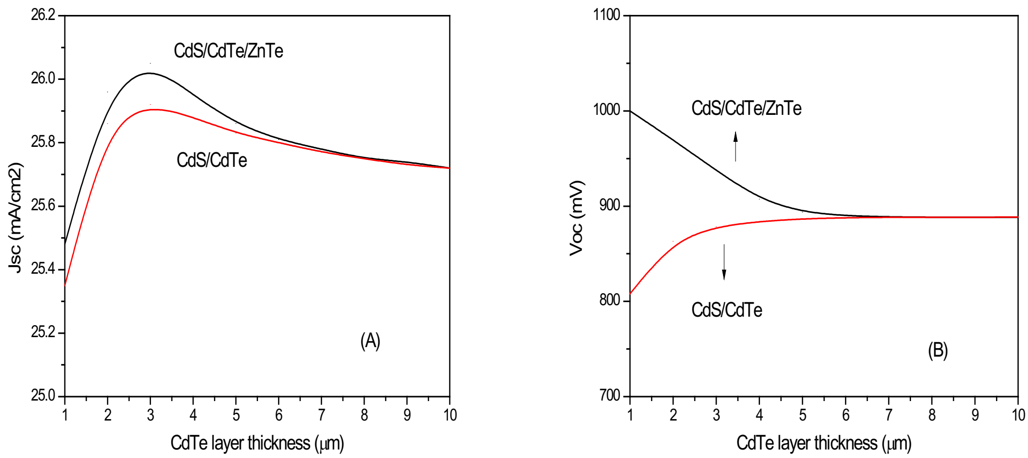

Fig. 5. (A) Short circuit current density (Jsc) and (B) Open circuit voltage (Voc) as a function of CdTe film thickness for $SnO_2/CdS/CdTe/ZnTe$ as compared to the conventional $SnO_2/CdS/CdTe$ structure.

It can be seen in fig. 5 (for simplicity only Jsc and Voc are shown) that the expected higher efficiency for the CdS/CdTe/ZnTe, as compared to the conventional solar cell, is a result mainly of the higher open circuit voltage as the thickness is reduced below 1 μm. This effect, as discussed above, is due both to the back surface and to the built-in electric fields in the CdTe layer, as a consequence of the back ZnTe layer in the former case.

Notice that the above results do not contradict the prediction by the author that with a conventional solar cell it would not be possible to have efficiencies above 18% as shown in fig. 2. The author himself has suggested the use of a variable band-gap material with an appropriate profile in order to achieve higher efficiencies [12]. Such band-gap engineering can be done by grading the Zn (Cd) content in CdZnTe to be used as a new semiconductor absorbing layer instead of pure CdTe. The present work can be considered as a particular case of the suggested CdZnTe band-gap engineering. In other words, having a CdZnTe layer with an appropriate Zn (Cd) concentration profile should cause a higher efficiency as we expect to show in a future work. In the latter case, the ZnTe layer would always be the back layer material where the back contact will be made with all the benefits already shown.

3. CONCLUSIONS

We have shown that it is possible to make very thin CdS/CdTe/ZnTe solar cells with high efficiencies, above 19.5% as compared to conventional CdS/CdTe solar cells with expected efficiencies below 18%. The results imply that including the back ZnTe layer will allow higher efficiencies with a thinner (1 μm) CdTe layer. These results are attributed to effects due to the presence of the higher band-gap p+ ZnTe layer at the back. This layer will cause reduced carrier recombination at the back contact due to the barrier (conduction band discontinuity) for electrons at the interface between the CdTe and the ZnTe layers (back surface field). Then, the electrons will be reflected at this interface and they will be collected with a higher probability at the CdS/CdTe hetero-junction. In addition, due to the p+ character of the ZnTe layer, the solar cell will behave as a n-i-p device with a high open circuit voltage since -in this case- it will be determined by the total potential difference between the CdS and the ZnTe layers. This effect will also be related to the presence of a high electric field in the whole CdTe region, and this field will be higher as this layer thickness is reduced. Minority carriers will be drifted by this high electric field towards the CdS/CdTe junction, increasing their collection probability. An additional benefit of this layer would be a reduced specific contact resistivity when making the solar cells. Hence, a ZnTe back layer should be studied experimentally, as a way of improving the efficiency of CdS/CdTe solar cells (above 19.5%) at the same time that their thickness is made thinner (reduced solar cell cost).

Acknowledgements

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